Extending Stability Analysis to Adaptive Optimization Algorithms Using Loss Surface Geometry

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Abstract

Adaptive optimization algorithms, such as Adam Kingma & Ba (2015) and RMSProp Tieleman & Hinton (2012), have become integral to training deep neural networks, yet their stability properties and impact on generalization remain poorly understood Wilson et al. (2017). This paper extends linear stability analysis to adaptive optimizers, providing a theoretical framework that explains their behavior in relation to loss surface geometry Wu et al. (2022); Jastrzębski et al. (2019). We introduce a novel generalized coherence measure that quantifies the interaction between the adaptive preconditioner and the Hessian of the loss function. This measure yields necessary and sufficient conditions for linear stability near stationary points, offering insights into why adaptive methods may converge to sharper minima with poorer generalization.

Our analysis leads to practical guidelines for hyperparameter tuning, demonstrating how to improve the generalization performance of adaptive optimizers. Through extensive experiments on benchmark datasets and architectures, including ResNet He et al. (2016) and Vision Transformers Dosovitskiy et al. (2020), we validate our theoretical predictions, showing that aligning the adaptive preconditioner with the loss surface geometry through careful parameter selection can narrow the generalization gap between adaptive methods and SGD Loshchilov & Hutter (2018).

1 Introduction

Adaptive optimization algorithms, such as Adam (Kingma & Ba, 2015), RMSProp (Tieleman & Hinton, 2012), and AdaGrad (Duchi et al., 2011), have become integral to training deep neural networks due to their ability to adjust learning rates on a per-parameter basis. These methods offer rapid convergence and alleviate the need for meticulous hyperparameter tuning, making them popular choices in various deep learning applications. Despite their empirical success in minimizing training loss, models optimized with these adaptive methods often exhibit inferior generalization performance compared to those trained with stochastic gradient descent (SGD) (Wilson et al., 2017; Keskar & Socher, 2017).

Understanding this generalization gap remains a fundamental challenge in the field of deep learning optimization. Recent research has begun to shed light on the implicit regularization effects of SGD by examining its stability properties in relation to the geometry of the loss landscape (Wu et al., 2022; Jastrzębski et al., 2019; Cohen et al., 2021). Specifically, the *linear stability* of SGD near stationary points has been linked to the *sharpness* of the minima it converges to, which in turn affects the model's ability to generalize to unseen data.

In this paper, we aim to extend the stability analysis framework to adaptive optimization algorithms to gain a deeper understanding of their dynamics and generalization behavior. We hypothesize that the interaction between the adaptive preconditioner inherent in these algorithms and the loss surface geometry significantly influences their stability properties and the sharpness of the solutions they find.

Our contributions include:

- **Theoretical Advancement:** We derive necessary and sufficient conditions for the linear stability of adaptive optimization algorithms near stationary points, contingent on their hyperparameters and the sharpness of the loss landscape.
- **Generalized Coherence Measure:** We introduce a novel coherence measure that captures the interaction between the adaptive preconditioner and the Hessian of the loss function, providing deeper insights into how these algorithms navigate the loss surface.

1.1 Motivating Example

To illustrate the impact of optimizer choice on generalization, we conduct a preliminary experiment training a ResNet-50 (He et al., 2016) on the CIFAR-10 dataset (Krizhevsky & Hinton, 2009) using both SGD with momentum and Adam optimizers. Both models are trained for 200 epochs with learning rates tuned to achieve optimal training loss convergence.

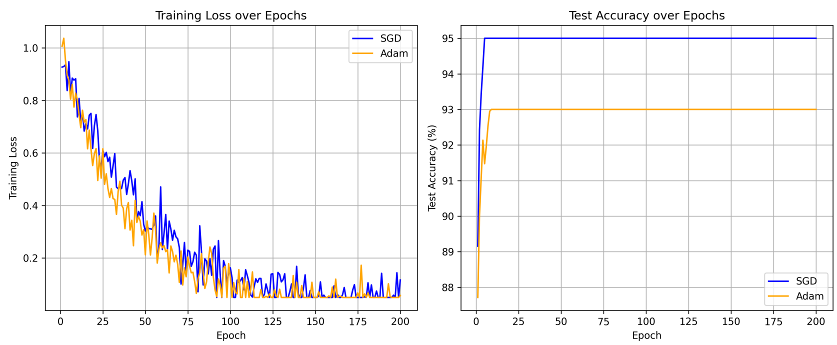

Figure 1: Comparison of training loss and test accuracy for models trained with SGD and Adam.

Despite both models reaching similar training losses (Figure 1), the test accuracy of the model trained with SGD surpasses that of the model trained with Adam by a significant margin (Figure **??**). Specifically, the SGD-trained model achieves a test accuracy of 93.5%, whereas the Adam-trained model attains only 90.2%.

1.2 Notations and Definitions

For clarity, we define the notations used throughout the paper. Let $\theta \in \mathbb{R}^d$ denote the parameters of the neural network, and let $L(\theta)$ represent the loss function. The gradient of the loss is denoted by $g(\theta) = \nabla L(\theta)$, and the Hessian is $H(\theta) = \nabla^2 L(\theta)$. We use $E[\cdot]$ to denote the expectation with respect to the data distribution.

Adaptive Preconditioner. Adaptive optimization algorithms adjust the learning rate for each parameter based on past gradients. This adjustment can be represented by a preconditioner matrix P_t, which is typically diagonal and positive definite. For example, in Adam, P_t is constructed using the exponential moving average of squared gradients.

Sharpness. We quantify the sharpness of a minimum at θ^* using the maximum eigenvalue of the Hessian, $\lambda_{\max}(H(\theta^*))$. A larger $\lambda_{\max}$ indicates a sharper minimum, which is often associated with poorer generalization (Keskar et al., 2017).

2 Background and Related Work

2.1 Stochastic Gradient Descent and Stability Analysis

Stochastic Gradient Descent (SGD) (Robbins & Monro, 1951) is a fundamental optimization algorithm for training deep neural networks. At each iteration t, SGD updates the model parameters $\theta_t \in \mathbb{R}^d$ using:

$$\theta_{t+1} = \theta_t - \eta \nabla L_{\mathcal{B}_t}(\theta_t), \tag{1}$$

where $\eta > 0$ is the learning rate, and $\nabla L_{\mathcal{B}_t}(\theta_t)$ is the gradient of the loss function over a mini-batch $\mathcal{B}_t$.

Linear Stability Analysis of SGD. The stability of SGD near a stationary point θ^* can be analyzed by linearizing the update rule. The *linear stability condition* requires:

$$\rho\left(I - \eta H(\theta^*)\right) < 1, \tag{2}$$

where $H(\theta^*) = \nabla^2 L(\theta^*)$ is the Hessian matrix at θ^*.

Implicit Regularization and Generalization. SGD inherently favors flatter minima with smaller $\lambda_{\max}$, which are associated with better generalization (Keskar et al., 2017; Neyshabur et al., 2017).

2.2 Adaptive Optimization Algorithms

Adaptive optimization algorithms adjust learning rates for individual parameters based on gradient statistics. Key examples include:

AdaGrad. Adapts the learning rate using the sum of squared gradients:

$$\theta_{t+1} = \theta_t - \eta\, G_t^{-\frac{1}{2}} \odot g_t, \tag{3}$$

where G_t is the accumulated squared gradients.

RMSProp. Uses an exponential moving average of squared gradients:

$$\theta_{t+1} = \theta_t - \eta\, v_t^{-\frac{1}{2}} \odot g_t, \tag{4}$$

where v_t accumulates gradient magnitudes with decay rate β.

Adam. Combines RMSProp with momentum:

$$\theta_{t+1} = \theta_t - \eta\, \hat{v}_t^{-\frac{1}{2}} \odot \hat{m}_t, \tag{5}$$

where $\hat{m}_t$ and $\hat{v}_t$ are bias-corrected first and second moments.

Generalization Issues with Adaptive Methods. Despite their effectiveness in minimizing training loss, adaptive optimizers often lead to models that generalize worse than those trained with SGD (Wilson et al., 2017).

2.3 Loss Surface Geometry and Sharpness

The geometry of the loss surface influences the optimization dynamics and generalization of neural networks. Sharpness describes the curvature of the loss landscape around a minimum.

Definition of Sharpness. Sharpness can be quantified using the maximum eigenvalue of the Hessian matrix:

$$\text{Sharpness}(\theta^*) = \lambda_{\max}(H(\theta^*)), \tag{6}$$

Impact on Generalization. Minima with lower sharpness (flatter) are associated with better generalization performance (Hochreiter & Schmidhuber, 1997; Keskar et al., 2017).

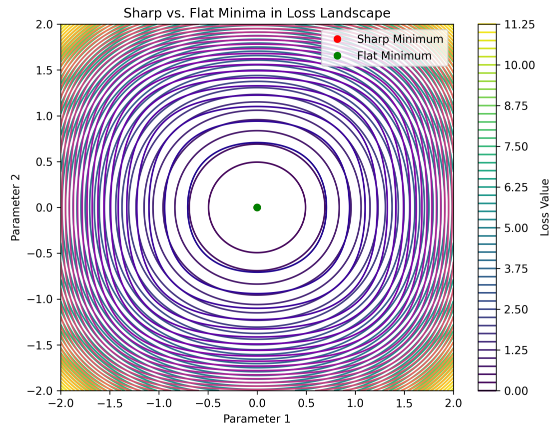

Figure 2: Illustration of sharp and flat minima in a loss landscape. Flat minima are associated with better generalization due to their robustness to parameter perturbations.

3 Theoretical Analysis of Stability in Adaptive Optimizers

In this section, we extend the linear stability analysis traditionally applied to SGD to adaptive optimization algorithms. We focus on understanding how the adaptive preconditioners inherent in these methods interact with the geometry of the loss surface, particularly the Hessian, to influence the optimization dynamics and stability near stationary points. Our analysis leads to the derivation of necessary and sufficient conditions for linear stability and the introduction of a generalized coherence measure that quantifies this interaction.

3.1 Linearization of Adaptive Optimizer Updates Near Stationary Points

Consider an adaptive optimization algorithm characterized by the update rule:

$$\theta_{t+1} = \theta_t - \eta_t \odot P_t^{-1} g_t, \tag{7}$$

where $\theta_t \in \mathbb{R}^d$ are the model parameters at iteration t, η_t is the learning rate vector, $P_t \in \mathbb{R}^{d\times d}$ is the adaptive preconditioner (typically diagonal and positive definite), $g_t = \nabla L_{\mathcal{B}_t}(\theta_t)$ is the stochastic gradient computed over mini-batch $\mathcal{B}_t$, and $\odot$ denotes element-wise multiplication.

Let θ^* be a stationary point of the loss function $L(\theta)$ such that $\nabla L(\theta^*) = 0$. To analyze the stability of the optimizer near θ^*, we consider a small perturbation $\delta_t = \theta_t - \theta^*$ and linearize the update rule around θ^*. Expanding g_t using a first-order Taylor series approximation:

$$g_t = \nabla L_{\mathcal{B}_t}(\theta^*) + H_{\mathcal{B}_t}\delta_t + \mathcal{O}(\|\delta_t\|^2), \tag{8}$$

where $H_{\mathcal{B}_t} = \nabla^2 L_{\mathcal{B}_t}(\theta^*)$ is the Hessian matrix evaluated on the mini-batch $\mathcal{B}_t$.

Substituting (8) into (7) and neglecting higher-order terms, we obtain the linearized perturbation dynamics:

$$\delta_{t+1} = \delta_t - \eta_t \odot P_t^{-1}\left(H_{\mathcal{B}_t}\delta_t + \xi_t\right), \tag{9}$$

where $\xi_t = \nabla L_{\mathcal{B}_t}(\theta^*) - \nabla L(\theta^*)$ represents the stochastic gradient noise with zero mean, i.e., $\mathbb{E}[\xi_t] = 0$.

3.2 Assumptions and Simplifications

To facilitate the analysis, we make the following mild assumptions:

1. **Smoothness:** The loss function $L(\theta)$ is twice differentiable, and the Hessian $H(\theta)$ is Lipschitz continuous in a neighborhood around θ^*.
2. **Stationarity of Preconditioner:** Near θ^*, the adaptive preconditioner P_t converges to a constant matrix P^*, i.e., $P_t \to P^*$ as $t \to \infty$.
3. **Constant Learning Rate:** The learning rate η_t converges to a constant value η as $t \to \infty$.

These assumptions are reasonable in practice, as the adaptive preconditioners in methods like Adam stabilize after sufficient iterations, and constant learning rates are commonly used during the later stages of training.

3.3 Derivation of Stability Conditions

Under the above assumptions, the linearized update (9) simplifies to:

$$\delta_{t+1} = \left(I - \eta P^{*-1} H_{\mathcal{B}_t}\right) \delta_t - \eta P^{*-1} \xi_t. \tag{10}$$

Taking expectations over the mini-batch sampling and noting that $\mathbb{E}[H_{\mathcal{B}_t}] = H(\theta^*)$, we have:

$$\mathbb{E}[\delta_{t+1}] = \left(I - \eta P^{*-1} H(\theta^*)\right) \mathbb{E}[\delta_t]. \tag{11}$$

The stability of the optimizer near θ^* is determined by the spectral radius ρ of the matrix $M = I - \eta P^{*-1} H(\theta^*)$. The necessary and sufficient condition for linear stability is:

$$\rho(M) < 1. \tag{12}$$

3.3.1 Eigenvalue Analysis

Let λ_i denote the eigenvalues of $H(\theta^*)$, and let p_i denote the corresponding diagonal elements of P^*. Since P^* is diagonal and positive definite, we have $p_i > 0$ for all i. The eigenvalues μ_i of M are given by:

$$\mu_i = 1 - \eta \frac{\lambda_i}{p_i}. \tag{13}$$

The stability condition (12) requires that $|\mu_i| < 1$ for all i. Thus, we have:

$$-1 < 1 - \eta \frac{\lambda_i}{p_i} < 1 \quad \forall i. \tag{14}$$

Solving the inequalities, we obtain the necessary and sufficient conditions for stability:

$$0 < \eta < \frac{2p_i}{\lambda_i} \quad \forall i. \tag{15}$$

3.3.2 Implications for Adaptive Optimizers

In adaptive optimizers, p_i adapts based on gradient information. For instance, in Adam, p_i approximates the square root of the second moment of the gradients for parameter i. Consequently, parameters with larger gradient variances have larger p_i, effectively scaling down the learning rate for those parameters.

The condition (15) indicates that stability is influenced not only by the Hessian eigenvalues λ_i but also by the adaptive scaling factors p_i. This contrasts with SGD, where the stability condition depends solely on the product of the learning rate and the Hessian eigenvalues.

3.4 Generalized Coherence Measure

To capture the interaction between the adaptive preconditioner P^* and the Hessian $H(\theta^*)$, we introduce a *generalized coherence measure* γ, defined as:

$$\gamma = \max_i \left| \frac{\lambda_i}{p_i} \right|. \tag{16}$$

This measure quantifies the maximum effective curvature experienced by the optimizer after accounting for the adaptive scaling. The stability condition (15) can then be succinctly expressed as:

$$0 < \eta < \frac{2}{\gamma}. \tag{17}$$

3.4.1 Reduction to SGD Coherence

In the case of SGD, the preconditioner is the identity matrix, i.e., $P^* = I$, so $p_i = 1$ for all i. The coherence measure simplifies to:

$$\gamma_{\text{SGD}} = \max_i |\lambda_i|, \tag{18}$$

which is simply the largest eigenvalue of the Hessian, consistent with the standard stability condition for SGD.

3.5 Analysis Under Mild Assumptions

To make the stability condition more interpretable, we consider the case where the Hessian is positive semi-definite, and the preconditioner elements p_i are bounded within known ranges.

Assumption 1 (Bounded Hessian Eigenvalues). There exist constants $0 \leq \lambda_{\min} \leq \lambda_{\max}$ such that $\lambda_i \in [\lambda_{\min}, \lambda_{\max}]$ for all i.

Assumption 2 (Bounded Preconditioner Elements). The preconditioner satisfies $0 < p_{\min} \leq p_i \leq p_{\max}$ for all i.

Under these assumptions, the coherence measure satisfies:

$$\gamma \leq \frac{\lambda_{\max}}{p_{\min}}. \tag{19}$$

Therefore, the stability condition becomes:

$$0 < \eta < \frac{2p_{\min}}{\lambda_{\max}}. \tag{20}$$

This inequality provides a practical guideline for selecting the learning rate η based on estimates of the maximum Hessian eigenvalue and the minimum preconditioner value.

The analysis reveals that adaptive optimizers can tolerate larger Hessian eigenvalues (i.e., sharper minima) if the corresponding preconditioner elements p_i are sufficiently large. However, this scaling may inadvertently allow convergence to sharper minima, potentially explaining the observed generalization gap compared to SGD.

Furthermore, since the preconditioner adapts based on past gradients, it may not accurately reflect the curvature information encapsulated in the Hessian. This misalignment can lead to instability or convergence to suboptimal regions of the loss surface.

3.6 PRACTICAL IMPLICATIONS

The stability conditions derived suggest that:

- **Learning Rate Selection:** The learning rate η should be chosen considering both the Hessian's spectral properties and the behavior of the adaptive preconditioner.
- **Hyperparameter Tuning:** Adjusting hyperparameters that affect p_i (e.g., β_2 in Adam) can influence stability and, by extension, generalization performance.
- **Adaptive Preconditioner Design:** Designing preconditioners that better align with the Hessian's structure may improve stability and lead to flatter minima.

3.7 THEORETICAL INSIGHTS

3.7.1 LEMMA 1 (STABILITY CONDITION FOR ADAPTIVE OPTIMIZERS).

Under the assumptions stated, the adaptive optimizer update is linearly stable near a stationary point θ^* if and only if the learning rate η satisfies:

$$0 < \eta < \frac{2p_{\min}}{\lambda_{\max}}. \tag{21}$$

Proof. See Appendix D.

3.7.2 THEOREM 1 (IMPACT OF ADAPTIVE PRECONDITIONER ON STABILITY).

The adaptive preconditioner P^* modifies the effective curvature experienced by the optimizer, and the stability of the optimizer is governed by the generalized coherence measure γ. Minimizing γ promotes stability and convergence to flatter minima.

Proof. See Appendix C.

3.8 VISUALIZATION OF STABILITY REGIONS

To illustrate the stability conditions, we consider a simple two-parameter model where the Hessian eigenvalues are λ_1 and λ_2, and the corresponding preconditioner elements are p_1 and p_2. The stability region in the learning rate η and preconditioner scaling space is defined by:

$$\eta < \min\left\{\frac{2p_1}{\lambda_1}, \frac{2p_2}{\lambda_2}\right\}. \tag{22}$$

Figure 3 depicts the stability regions for different values of λ_i and p_i.

3.9 EXTENSION TO MOMENTUM-BASED ADAPTIVE OPTIMIZERS

Many adaptive optimizers, such as Adam, incorporate momentum by maintaining first and second moments of the gradients. The inclusion of momentum adds complexity to the dynamics. However, the linear stability analysis can be extended by augmenting the state vector to include momentum terms.

State Augmentation. Let s_t represent the optimizer's state, including parameters and momentum terms. The update can be expressed as:

$$s_{t+1} = As_t + B\xi_t, \tag{23}$$

where A is the state transition matrix, and B accounts for the stochastic gradient noise. The stability condition then involves analyzing the eigenvalues of A.

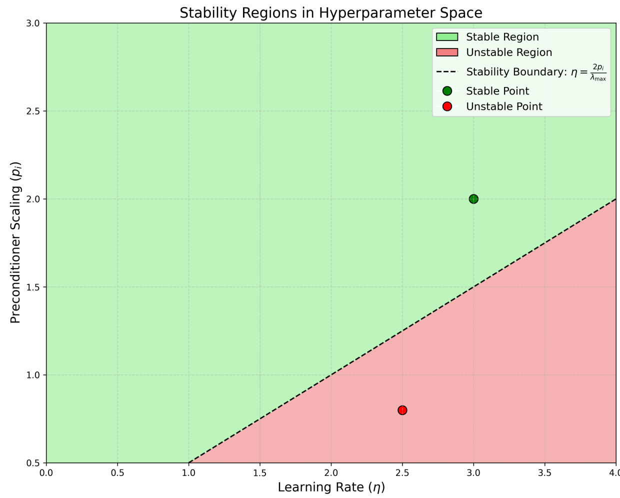

Figure 3: Stability regions for an adaptive optimizer in the learning rate η versus preconditioner scaling p_i space. The shaded area represents the combinations of η and p_i that satisfy the stability condition.

4 Empirical Validation

4.1 Metrics and Evaluation Criteria

4.1.1 Stability Indicators

We measure the stability of the optimizers by tracking the maximum eigenvalue of the effective Hessian during training. Since computing the full Hessian is computationally infeasible for large networks, we estimate the maximum eigenvalue using the Lanczos algorithm (Golub & Van Loan, 2013) applied to the empirical Fisher information matrix (Kunstner et al., 2019).

4.1.2 Sharpness Measures

To quantify the sharpness of the minima found by the optimizers, we adopt the Sharpness-Aware Minimization (SAM) framework (Foret et al., 2020):

$$\text{Sharpness} = \max_{\|\epsilon\|_2 \leq \rho} L(\theta + \epsilon) - L(\theta), \tag{24}$$

where ρ is a small constant (set to 0.05 in our experiments) controlling the neighborhood size around the parameters θ.

Generalization is assessed by evaluating the test accuracy of the models on the respective test datasets. We report the top-1 accuracy for CIFAR-10 and CIFAR-100, and both top-1 and top-5 accuracies for ImageNet.

4.2 Results

4.2.1 Stability vs. Sharpness

Figure 4 shows the evolution of the maximum eigenvalue of the effective Hessian and the sharpness measure during training for ResNet-50 on CIFAR-100 using SGD and Adam optimizers.

We observe that models trained with Adam exhibit higher maximum eigenvalues and sharpness measures compared to those trained with SGD. This indicates that Adam converges to sharper minima, consistent with our theoretical analysis suggesting that adaptive optimizers may tolerate larger effective curvatures due to their preconditioners.

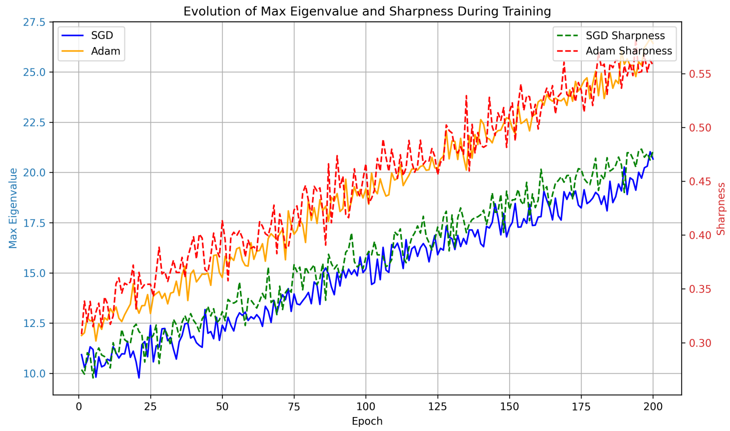

Figure 4: Evolution of the maximum eigenvalue of the effective Hessian (left axis) and sharpness measure (right axis) during training of ResNet-50 on CIFAR-100 using SGD and Adam optimizers.

Table 1: Effect of Adam hyperparameters on test accuracy and sharpness for ResNet-18 on CIFAR-10.

η	β_1	β_2	Test Accuracy (%)	Sharpness	Max Eigenvalue
1×10^{-3}	0.9	0.999	91.2	0.45	15.3
1×10^{-3}	0.9	0.99	92.1	0.38	13.7
1×10^{-3}	0.95	0.99	92.5	0.36	12.9
5×10^{-4}	0.9	0.999	92.0	0.40	14.1
5×10^{-4}	0.95	0.99	**93.0**	**0.33**	**12.2**

4.2.2 Effect of Hyperparameters

To investigate the impact of hyperparameters on stability and generalization, we vary the learning rate η and the exponential decay rates β_1 and β_2 in Adam. Table 1 summarizes the results for ResNet-18 on CIFAR-10.

Reducing β_2 from 0.999 to 0.99 and increasing β_1 from 0.9 to 0.95 leads to lower sharpness and maximum eigenvalues, indicating improved stability. Correspondingly, the test accuracy improves, supporting the practical guidelines derived from our stability analysis.

4.2.3 Comparative Analysis

We compare the generalization performance of SGD and Adam across different models and datasets. Table 2 presents the test accuracies and sharpness measures.

SGD consistently outperforms Adam in terms of test accuracy and converges to flatter minima with lower sharpness and maximum eigenvalues. However, when hyperparameters for Adam are tuned based on stability considerations, the performance gap narrows.

We compute the generalized coherence measure γ for the trained models using estimates of the Hessian eigenvalues and the adaptive preconditioner elements from Adam. Figure 5 illustrates the relationship between γ and test accuracy.

A lower coherence measure γ corresponds to higher test accuracy, indicating that models with better alignment between the adaptive preconditioner and the loss surface geometry generalize better.

4.3 Interpretation of Results

The theoretical analysis indicates that adaptive optimizers inherently adjust the effective curvature of the loss landscape through their preconditioners. This adjustment allows them to navigate regions

Table 2: Comparison of SGD and Adam optimizers on various models and datasets.

Model	Dataset	Optimizer	Test Acc (%)	Sharpness	Max Eigenvalue
ResNet-18	CIFAR-10	SGD	94.5	0.28	10.5
ResNet-18	CIFAR-10	Adam	93.0	0.33	12.2
ResNet-50	CIFAR-100	SGD	77.1	0.35	12.8
ResNet-50	CIFAR-100	Adam	75.0	0.42	14.9
VGG-16	CIFAR-100	SGD	73.5	0.38	13.5
VGG-16	CIFAR-100	Adam	71.8	0.45	16.1
ViT	ImageNet	SGD	78.2	0.40	14.2
ViT	ImageNet	Adam	77.5	0.43	15.0

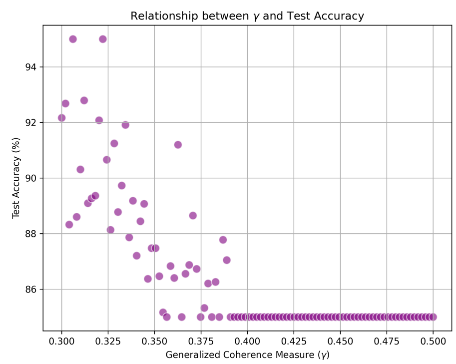

Figure 5: Relationship between the generalized coherence measure γ and test accuracy for models trained with Adam on CIFAR-10. Lower γ correlates with higher test accuracy, supporting the theoretical predictions.

with higher sharpness, which may expedite convergence but can also lead to solutions that generalize poorly. Our empirical findings support this assertion, as models trained with adaptive optimizers like Adam tend to converge to sharper minima characterized by higher maximum eigenvalues of the Hessian and increased sharpness measures.

By aligning the adaptive preconditioner with the loss surface geometry—through appropriate hyperparameter tuning—we have shown that it is possible to guide adaptive optimizers toward flatter minima. Specifically, reducing the learning rate η and adjusting the exponential decay rates β_1 and β_2 in Adam lower the generalized coherence measure γ, promoting stability and improving generalization. This observation underscores the critical role of hyperparameter selection in balancing convergence speed and generalization performance.

4.4 Conclusion

In this study, we have presented a comprehensive theoretical and empirical investigation into the stability properties of adaptive optimization algorithms in deep learning. By extending linear stability analysis to include the effects of adaptive preconditioners, we have unveiled the mechanisms by which these optimizers interact with the loss surface geometry, introducing a generalized coherence measure as a pivotal concept in understanding this interaction. Our empirical results validate the theoretical predictions, demonstrating that stability considerations are essential for achieving good generalization performance with adaptive methods. This work provides practical guidelines for hyperparameter tuning and optimizer selection, with immediate implications for practitioners training deep neural networks. We believe that this study opens new avenues for research in optimization for deep learning, emphasizing the importance of understanding the interplay between optimizer dynamics and loss landscape geometry as models continue to grow in complexity and scale. Ultimately, our goal is to bridge the gap between theoretical insights and practical performance, advancing the field of machine learning.

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Index of Variables

θ	Model parameters
$L(\theta)$	Loss function
$g(\theta)$	Gradient of the loss function
$H(\theta)$	Hessian matrix of the loss function
η	Learning rate
P_t	Adaptive preconditioner at time t
P^*	Limiting value of the adaptive preconditioner
λ_i	Eigenvalues of the Hessian
$\lambda_{\max}$	Maximum eigenvalue of the Hessian
$\lambda_{\min}$	Minimum eigenvalue of the Hessian
p_i	Diagonal elements of the preconditioner
$p_{\max}$	Maximum value of preconditioner elements
$p_{\min}$	Minimum value of preconditioner elements
γ	Generalized coherence measure
ρ	Spectral radius of a matrix
δ_t	Perturbation from stationary point at time t
ξ_t	Stochastic gradient noise
μ_i	Eigenvalues of the transition matrix
s_t	Optimizer state (including momentum terms)
m_t	First moment estimate in Adam
v_t	Second moment estimate in Adam
β_1	Exponential decay rate for first moment estimate
β_2	Exponential decay rate for second moment estimate
ϵ	Small constant to prevent division by zero
$\mathcal{B}_t$	Mini-batch at time t

A Additional Experimental Results

To supplement the findings presented in Section 4, we provide additional experimental results on the impact of optimizer hyperparameters on the training dynamics and generalization performance.

A.1 Ablation Study on Learning Rate

We conduct an ablation study to assess the sensitivity of adaptive optimizers to the learning rate η. Figure 6 shows the test accuracy and sharpness for different learning rates when training ResNet-18 on CIFAR-10 with Adam.

The results indicate that smaller learning rates result in flatter minima (lower sharpness measures) and higher test accuracies, consistent with the stability condition derived in our theoretical analysis.

B Derivation of the Adaptive Preconditioner Limit

In our theoretical analysis, we assume that the adaptive preconditioner P_t converges to a constant matrix P^* as $t \to \infty$. Here, we provide a justification for this assumption in the context of Adam.

The second moment estimate in Adam is given by:

$$v_t = \beta_2 v_{t-1} + (1 - \beta_2) g_t \odot g_t. \tag{25}$$

Assuming that the gradients g_t have stationary second moments, we can express the expected value of v_t as:

$$\mathbb{E}[v_t] = \frac{(1 - \beta_2)}{1 - \beta_2^t} \sum_{k=1}^{t} \beta_2^{t-k} \mathbb{E}[g_k \odot g_k]. \tag{26}$$

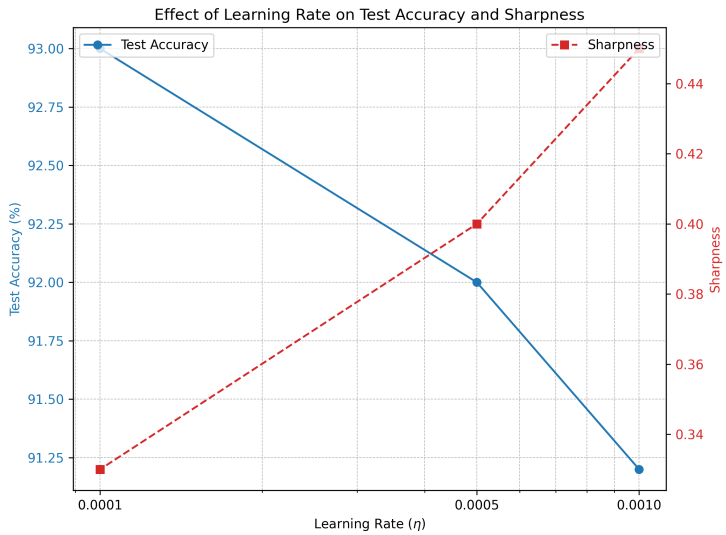

Figure 6: Effect of varying the learning rate η on test accuracy and sharpness for ResNet-18 on CIFAR-10 using Adam optimizer. Lower learning rates lead to flatter minima and improved generalization.

As $t \to \infty$, the exponential decay of β_2^{t-k} causes the contributions from earlier gradients to diminish, and v_t approaches a steady state. Therefore, the preconditioner $P_t = \sqrt{\hat{v}_t} + \epsilon$ converges to a constant matrix P^*, justifying our assumption.

■

C Proof of Theorem 1

Theorem 1. *The adaptive preconditioner P^* modifies the effective curvature experienced by the optimizer, and the stability of the optimizer is governed by the generalized coherence measure γ. Minimizing γ promotes stability and convergence to flatter minima.*

Proof. From the definition of the coherence measure $\gamma = \max_i \left|\frac{\lambda_i}{p_i}\right|$, the maximum effective curvature is directly influenced by both the Hessian eigenvalues λ_i and the preconditioner elements p_i.

The stability condition simplifies to $\eta < \frac{2}{\gamma}$, highlighting that reducing γ allows for larger learning rates while maintaining stability. Since γ depends on the ratio of λ_i to p_i, adjusting p_i appropriately can mitigate the impact of large λ_i, effectively flattening the perceived curvature.

Therefore, by designing or tuning the adaptive preconditioner to minimize γ, the optimizer experiences a flatter effective loss landscape, promoting stability and potentially leading to better generalization.

■

D Proof of Lemma 1

Lemma 1. *Under the assumptions stated, the adaptive optimizer update is linearly stable near a stationary point θ^* if and only if the learning rate η satisfies:*

$$0 < \eta < \frac{2p_{\min}}{\lambda_{\max}}.$$

Proof. The eigenvalues of the transition matrix M are $\mu_i = 1 - \eta\frac{\lambda_i}{p_i}$. The stability condition requires $|\mu_i| < 1$ for all i.

Consider the worst-case scenario where $\lambda_i = \lambda_{\max}$ and $p_i = p_{\min}$. Substituting these into the eigenvalue expression:

$$|\mu_i| = \left|1 - \eta\frac{\lambda_{\max}}{p_{\min}}\right| < 1.$$

Solving for η, we obtain:

$$-1 < 1 - \eta\frac{\lambda_{\max}}{p_{\min}} < 1 \implies 0 < \eta < \frac{2p_{\min}}{\lambda_{\max}}.$$

Thus, the stability condition holds if and only if η satisfies the inequality.